

Identifying the Effect of Non-Ideal Mixing on a Pre-Denitrification Activated Sludge System Performance through Model-Based Simulations

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Effectiveness of a pre-denitrification activated sludge treatment system is governed by the kinetics of the biological reactions, and the hydrodynamic mixing behavior in the reactors. Achieving good mixing conditions within a reactor not only enhances the transfer of reactants but also ensures homogeneous environmental conditions throughout the vessel when required, allowing for an effective usage of the reactor's total volume, leading to optimized, low-cost operation. In this work, a pre-denitrification activated sludge system performance with regards to the biological treatment of organic carbon and nitrogen was investigated, under two scenarios for non-ideal mixing in the anoxic reactor. The system performance is simulated based upon the Activated Sludge Model 1 model's biological reactions, and combining two non-ideal mixing two-parameter models: CSTR with bypass and dead volume, and two CSTRs with exchange. Performance discrepancies were then identified in the presence of non-ideal mixing. The system's performance was found to be more susceptible to the presence of a dead volume/bypass scenario compared to the two CSTRs with material exchange scenario. Under non-ideal mixing conditions, effluent concentrations of Total Kjeldahl Nitrogen, organic carbon increased marginally, while effluent concentration of nitrate increased significantly. Similarly, the waste stream concentrations of Total Kjeldahl Nitrogen and organic carbon increased significantly as a result of an increase in the concentration of the heterotrophic biomass. The outcome of this study provides an insight when troubleshooting the operation of pre-denitrification activated sludge systems for non-ideal mixing conditions.

Keywords: Non-ideal mixing, Activated sludge, Dead volume, Bypass, Material exchange

Introduction

Activated Sludge (AS) systems are among the most widely employed biological treatment processes in wastewater treatment plants (Rittmann and McCarty, 2001). AS systems are engineered processes, designed and operated to sustain and facilitate the growth of different microorganisms. These microorganisms in their part treat wastewaters biologically by incorporating/removing the pollutants in their different metabolic and growth associated processes. Those pollutants are mainly comprised of dissolved and particulate organic carbon and nitrogen-containing compounds. The main biological processes leading to wastewater treatment taking place in AS systems, and the associated microorganisms responsible for them are organic carbon mineralization under aerobic and anoxic conditions by facultative heterotrophic bacteria, ammonia (NH_3) oxidation under aerobic conditions to nitrate (NO_3^-) by autotrophic nitrifying bacteria, and nitrate reduction under anoxic conditions to nitrogen gas (N_2) by the aforementioned facultative heterotrophic bacteria (utilized instead of oxygen in the metabolic process) (Madigan and Martinko, 2006; Tchobanoglous *et al.*, 2007). Pre-denitrification is (PD) one approach for the operation of AS (Hellinga *et al.*, 1999; Kim *et al.*, 2009). The required environmental conditions (anoxic and aerobic) are divided between two distinctive Continuous-flow stirred-tank reactors (CSTRs), and the microorganisms (biomass) are circulated between them. **Figure 1**, illustrates the process scheme. The anoxic reactor receives both fresh organic carbon and ammonia containing wastewater and a nitrate-rich, biomass containing, mixed liquor recycle from the aerobic reactor, where a portion of organic carbon is mineralized and nitrate is reduced to nitrogen gas. Anoxic reactor effluent carries the remaining untreated wastewater to the aerobic reactor, where air is supplied to sustain an elevated oxygen concentration, and enhanced mixing conditions. The remaining organic carbon is completely mineralized and ammonia is oxidized to nitrate. The settler allows for biomass to be separated from the mixed liquor, and recycled back so that the system's solids retention time is controlled independently from the system's hydraulic retention time (Tchobanoglous *et al.*, 2007). Effectiveness of a PD-AS treatment system is governed by the kinetics of the biological reactions, and the hydrodynamics of mixing in the reactors. The different reactions and processes taking place in a PD-AS system were first identified and modeled by the International Water Association (IWA) Activated Sludge Model 1 (ASM1) (Henze *et al.*, 2000), and since employed in a wide variety of studies (Alex *et al.*, 2008; Hajaya and Pavlostathis, 2013; Ostace *et al.*, 2011; Van Loosdrecht *et al.*, 2015). Ideal mixing conditions are commonly assumed while designing biological reactors for wastewater treatment processes (Vanrolleghem *et al.*, 2003). Achieving good mixing conditions within reactors not only enhances the transfer of substrates (reactants) but also ensures homogeneous environmental conditions throughout the vessel, thereby, allowing for an effective usage of the reactor's total volume leading to optimized and low-cost operation (Badkoubi *et al.*, 1998; García *et al.*, 2005).

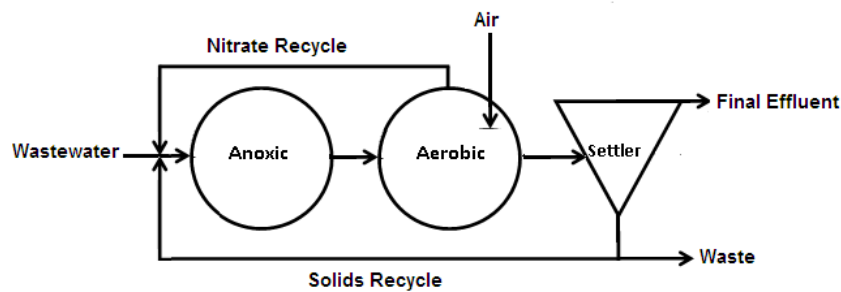


Fig. 1 Typical pre-denitrification activated sludge system including anoxic and aerobic reactors and settler

Despite the assumption of ideal mixing in biological reactors, it is likely non-ideal mixing conditions will prevail in the real situation. Kjellstrand (2006) studied the hydraulic behavior of a denitrifying activated sludge tank, located at the Rya Wastewater treatment plant (WWTP) in Göteborg Sweden, where it was found that up to 30% of the feed had notably fast hydraulic retention times, while up to 21% of the feed had notably slow hydraulic retention times compared to the nominal hydraulic retention time. This indicated the presence of feed bypass and stagnation zones in the system. Sánchez and coworkers (Sánchez *et al.*, 2016) performed the hydraulic characterization for the secondary treatment system in the WWTP of San Pedro del Pinatar. They reported that only 70.5% of the system's volume was active, while the remaining 29.5% was actually a dead volume. Collivignarelli and coworkers (Collivignarelli *et al.*, 2018) reported a dead volume fractions ranging from 15% to 25%, and bypass fractions ranging between 35% and 40%, while performing the experimental verification of reactor hydrodynamics for an undisclosed WWTP. Manenti and coworkers (Manentiet *et al.*, 2018) have identified a 5% fraction of dead volume in a pilot-scale WWTP. Non-ideal mixing occurrences in AS systems were reported for constructed, operational wastewater treatment plants, which could be brought by poor design or equipment failure. The cost of diagnosing their presence in such systems could be drastically reduced if mathematical simulations are used. The purpose of this work is to identify the possible consequences of non-ideal mixing on the biological processes performance. Such discrepancies in performance can be used in identifying the presence of non-ideal mixing behavior in the AS system reactors. In this work, a pre-denitrification activated sludge (PD-AS) unit performance with regards to the biological treatment of organic carbon and nitrogen is investigated under the conditions of non-ideal mixing in the anoxic reactor. The system performance is simulated based upon the ASM1 model's biological reactions (Henze *et al.*, 2000), and combining two non-ideal mixing two-parameter models: CSTR with bypass and dead volume, and two CSTRs with exchange (Fogler, 1999). Performance discrepancies could then be identified by comparing the performance of the system under non-ideal mixing to performance of the system at ideal mixing conditions.

1 Mathematical Models

1.1 Biological reactions

The ASM1 model identified the specific processes in PD-AS to be: aerobic growth of heterotrophs, anoxic growth of heterotrophs, aerobic growth of autotrophs, decay of heterotrophs, decay of autotrophs, ammonification of soluble organic nitrogen, hydrolysis of entrapped organics, and hydrolysis of entrapped organic nitrogen (Henze *et al.*, 2000). **Tables 1** detail each process mathematical model, where S denotes the soluble constituents' concentrations, and X denotes particulate constituents' concentrations, while **Table 2** lists the different variables associated with the aforementioned processes, with the kinetics of each step involved in the PD-AS system.

1.2 Ideal completely mixed reactors model

Figure 2 shows the PD-AS system. In this work, both the widely adapted COAST benchmark and BSM1 benchmark (Alex *et al.*, 2008; Copp, 2002) are used for system size, albeit with some modifications. The system is designed for an average wastewater flow rate (Q) of 18400 m³/day, with ≈ 300 mg COD/L of biodegradable organic carbon and ≈ 50 mg N/L of nitrogen. Volumes of the anoxic and aerobic reactors are 2000 m³ (V_1) and 4000 m³ (V_2), respectively, with nitrate, recycle ratio (R_1) and solids recycle ratio (R_2) of 3 and 1, respectively. The waste flow rate (Q_w) is chosen for a 16-day SRT to be at 385 m³/day. Air is only introduced into the aerobic reactor to sustain an oxygen concentration of 2.1 ± 0.11 mg/l. The settler sub-model is not included in the system, and it is assumed that no reactions are taking place in it; instead, a particulates separation coefficient (SE) is assumed and used to calculate the concentration in the settler overflow (final effluent) and underflow. Particulate concentration (X) in both the settler's overflow (X_{OF}) and underflow (X_{UF}) is determined by mass balance around the settler, by using a settling efficiency (SE), which is assumed constant (Le Moullec *et al.*, 2011) and can be defined as $SE = \text{Particulate mass in the underflow} / \text{Particulate mass in the overflow}$:

$$X_{UF} = [SE \cdot Q \cdot X_2 \cdot (R_2 + 1)] / [R_2 \cdot Q + Q_W] \dots \quad (1)$$

$$X_{OF} = [(1 - SE) \cdot Q \cdot X_2 \cdot (R_2 + 1)] / [Q + Q_W] \dots \quad (2)$$

where X_2 is particulate concentration (mg COD/l) in the aerobic reactor.

Table 1 Biological processes taking place in the PD-AS, adapted from the ASM1 model (Henze *et al.*, 2000)

Process	Model	Symbol
Aerobic growth of heterotrophs	$\mu_H \frac{S_s}{S_s + K_s} \frac{S_O}{S_O + K_{OH}} X_{BH}$	P_1
Anoxic growth of heterotrophs	$\mu_H \frac{S_s}{S_s + K_s} \frac{K_{OH}}{S_O + K_{OH}} \frac{S_{NO}}{S_{NO} + K_{NO}} \eta_G X_{BH}$	P_2
Aerobic growth of autotrophs	$\mu_A \frac{S_{NH}}{S_{NH} + K_s} \frac{S_O}{S_O + K_{OA}} X_{BA}$	P_3
Decay of heterotrophs	$b_H X_{BH}$	P_4
Decay of autotrophs	$b_A X_{BA}$	P_5
Ammonification of soluble organic nitrogen	$k_a S_{ND} X_{BH}$	P_6
Hydrolysis of entrapped organics	$k_h \frac{X_s/X_{BH}}{X_s/X_{BH} + K_X} \left[\frac{K_{OH}}{S_O + K_{OH}} + \eta_h \frac{S_{NO}}{S_{NO} + K_{NO}} \frac{K_{OH}}{S_O + K_{OH}} \right] X_{BH}$	P_7
Hydrolysis of entrapped organic nitrogen	$P_7 \frac{X_{ND}}{X_s}$	P_8

Table 2 State variables in the PD-AS model and their associated rates

Variable	Definition	Rate
S_I^a	Soluble inert organics	$r_{SI} = 0$
S_S^a	Readily biodegradable (soluble) substrate	$r_{SS} = \frac{-1}{y_H} (P_1 + P_2) + P_7$
X_I^a	Particulate inert organics	$r_{XI} = 0$
X_S^a	Slowly biodegradable (particulate) substrate	$r_{XS} = (1 - f_p)(P_4 + P_5) - P_7$
X_{BH}^a	Active heterotrophic biomass	$r_{XBH} = P_1 + P_2 - P_4$
X_{BA}^a	Active autotrophic biomass	$r_{XBA} = P_3 - P_5$
X_P^a	Non-biodegradable particulates	$r_{XP} = f_p(P_4 + P_5)$
S_O^b	Dissolved oxygen	$r_{SO} = -\frac{1 - y_H}{y_H} P_1 - \frac{4.57 - y_A}{y_A} P_3$
S_{NO}^c	Nitrate	$r_{SNO} = \frac{1 - y_H}{2.86 y_H} P_2 + \frac{1}{y_A} P_3$
S_{NH}^c	Free and ionized ammonia	$r_{SNH} = \left(-i_{XB} - \frac{1}{y_A} \right) P_3 - i_{XB} (P_1 + P_2) + P_6$
S_{ND}^c	Soluble biodegradable organic nitrogen	$r_{SND} = P_8 - P_6$
X_{ND}^c	Particulate biodegradable organic N	$r_{XND} = (i_{XB} - i_{XP} f_p)(P_4 + P_5) - P_8$
S_{ALK}^d	Alkalinity	$r_{SALK} = P_7 \frac{X_{ND}}{X_s}$

a: mg COD/L; mg of Chemical Oxygen Demand; b: mg O_2 /L; c: mg N/L; d: mol/L.

Assuming ideal CSTR behavior in the anoxic and aerobic reactors, constant liquid densities and reactor volumes, and reactions taking place only in the reactors, the following equations can be used to describe the dynamic behavior of soluble (S) and particulate constituents:

For the anoxic reactor:

$$dS_1/dt = (Q/V_1) ([S_i + S_2(R_1 + R_2)] - [1 + R_1 + R_2]S_1) + r_{S1} \dots \quad (3)$$

$$dX_1/dt = (Q/V_1) ([X_i + X_2 R_1 + X_{UF} R_2] - [1 + R_1 + R_2]X_1) + r_{X1} \dots \quad (4)$$

For the aerobic reactor:

$$dS_2/dt = (Q[1 + R_1 + R_2]/V_2) (S_1 - S_2) + r_{S2} \dots \quad (5)$$

$$dX_2/dt = (Q[1 + R_1 + R_2]/V_2) (X_1 - X_2) + r_{X2} \dots \quad (6)$$

Where S_1 and X_1 are the concentrations in the anoxic reactor, S and X_i are the concentrations in the feed wastewater (**Table 3**), and S_2 and X_2 are the concentrations in the aerobic reactor, respectively. X_{UF} is the particulate concentrations in the solids recycle (Equation 1), and $r_{S1\&S2}$ and $r_{X1\&X2}$ are the rates in the different reactors (Table 2). Finally for oxygen, in the aerobic reactor, the following rate is

introduced to represent the aeration rate (r_{Air-in}):

$$r_{Air-in} = K_L(S_O^{SAT} - S_{O2}) \quad (7)$$

where K_L is the oxygen transfer coefficient (d^{-1}) maintained at a level in the aerobic reactor to provide a constant oxygen concentration (as mentioned above) (Alex *et al.*, 2008), and S_O^{SAT} is oxygen saturation concentration = 8mg/L, (at 26°C and 1atm) (Rittmann and McCarty, 2001), and S_{O2} is the oxygen concentration in the aerobic reactor (mg/L).

1.3 Non-ideal mixing models

Among the PD-AS system reactors, the anoxic reactor is the most susceptible to the occurrence of non-ideal mixing. Mixing in this reactor is solely performed mechanically, compared to superior mixing conditions (minimizing non-ideal mixing) brought by the aeration process taking place in the aerobic reactor. Accordingly, the non-ideal mixing scenarios are assumed to affect the anoxic reactor in the PD-AS. Oxygen concentration and settler behavior are handled in the same matter as discussed above in the ideal CSTR based system.

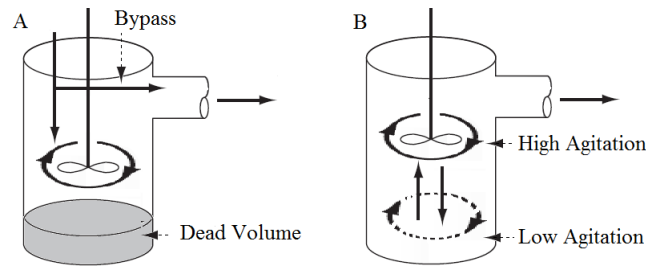


Fig. 2 Non-ideal, real mixing scenarios; A: Bypass with dead volume, and B: Rapid and slow mixing.

1.3.1 CSTR with bypass and dead volume

In this situation, poor mixing results in generating a dead zone within the reactor volume, where limited or no exchange of material is taking place between it and the remaining reactor volume. This will reduce the available volume for reactions within the reactor itself. In addition, poor mixing can allow for a portion of the feed to exit rapidly without being mixed inside the reactor, as if that portion is totally not entering the reactor, but rather bypassing it directly to the effluent (**Figure 2.A**). Previous scenarios are modeled as a combination of an ideal CSTR coupled with a dead zone. These volumes are defined as fractions of the total reactor volume (V), where $\alpha = \text{volume of CSTR}/V$ and $(1-\alpha) = \text{volume of dead zone}/V$. On the other hand, flow rates headed for the reactor (Q) have a fraction that bypasses it while the remaining fraction enters it, where $\beta = \text{bypassed flow}/Q$ and $(1-\beta) = \text{entering flow}/Q$ (Fogler, 1999). The degree of nonideality depends on the values of α and β . The presence of a bypass and a dead volume in real engineered biological reactors has been previously reported (Collivignarelli *et al.*, 2018; Kjellstrand, 2006; Manenti *et al.*, 2018; Sánchez *et al.*, 2016). In light of the previous argument, the dynamic behavior of soluble and particulate constituents in both reactors no longer behaves as described by Equations 3, 4, 5, and 6. Assuming constant values for α , β (for all streams entering), liquid densities and reactor volumes, and reactions taking place only in the reactors, the following equations can be used to describe the dynamic behavior of soluble and particulate constituents:

For the anoxic reactor:

$$dS_1/dt = (Q(1-\beta)/\alpha V_1) ([S_i + S_2(R_1 + R_2)] - [1 + R_1 + R_2]S_1) + r_{S1} \dots \quad (8)$$

$$dX_1/dt = (Q(1-\beta)/\alpha V_1) ([X_i + X_2R_1 + X_{UF}R_2] - [1 + R_1 + R_2]X_1) + r_{X1} \dots \quad (9)$$

For the aerobic reactor:

$$dS_2/dt = (Q/V_2) ((1-\beta)[1 + R_1 + R_2]S_1 + \beta[S_i + S_2(R_1 + R_2)] - [1 + R_1 + R_2]S_2) + r_{S2} \dots \quad (10)$$

$$dX_2/dt = (Q/V_2) ((1-\beta)[1 + R_1 + R_2]X_1 + \beta[X_i + X_2R_1 + X_{UF}R_2] - [1 + R_1 + R_2]X_2) + r_{X2} \dots \quad (11)$$

1.3.2 Two CSTRs with material exchange

This scenario depicts a situation where mixing apparatus are poorly situated within the reactor, resulting in rapid mixing in their vicinity, while the remaining region undergoes mixing, albeit at a lesser rate. This situation will influence the distribution of material within the reactor, affecting the different reactions rates due to an uneven distribution of substrates (**Figure 2.B**). In this situation, it is assumed that the anoxic reactor volume (V) is split into two fractions: a fraction that undergoes high agitation ($\alpha = \text{highly agitated volume}/V$) and a fraction with low agitation ($(1-\alpha) = \text{volume with less agitation}/V$). Material is exchanged between the two-volume fractions by a ratio of the flows entering the reactor; $\beta = \text{material exchange flow rate}/Q$. Both the inlet and outlet flow is directed to and

from the highly agitated portion (Fogler, 1999). As with the previous model, the degree of nonideality depends on the values of α and β . The two CSTR with exchange model has been previously used to describe non-ideal mixing in different biological reactors (Le Moulec *et al.*, 2010; Le Moulec *et al.*, 2011; Pereira *et al.*, 2012). Assuming constant values for α , β (for all streams entering), liquid densities and reactor volumes, and reactions taking place only in the reactors, the following equations can be used to describe the dynamic behavior of soluble and particulate constituents:

For the anoxic reactor highly agitated fraction (concentrations are accented with 1):

$$dS_1^1/dt = (Q(1 + R_1 + R_2)/\alpha V_1) ([S_i + S_2(R_1 + R_2)/1 + R_1 + R_2] - S_1^1 + \beta(S_2^1 - S_1^1)) + r_{S_1^1} \dots \quad (12)$$

$$dX_1^1/dt = (Q(1 + R_1 + R_2)/\alpha V_1) ([X_i + X_2 R_1 + X_{UF} R_2]/1 + R_1 + R_2] - X_1^1 + \beta(X_2^1 - X_1^1)) + r_{X_1^1} \dots \quad (13)$$

For the anoxic reactor fraction with less agitated (concentrations are accented with 2):

$$dS_1^2/dt = (Q(1 + R_1 + R_2)\beta/(1 - \alpha)V_1) (S_1^1 - S_2^2) + r_{S_1^2} \dots \quad (14)$$

$$dX_1^1/dt = (Q(1 + R_1 + R_2)\beta/(1 - \alpha)V_1) (X_1^1 - X_2^2) + r_{X_1^2} \dots \quad (15)$$

For the aerobic reactor:

$$dS_2/dt = (Q(1 + R_1 + R_2)/V_2) (S_1^1 - S_2) + r_{S_2} \dots \quad (16)$$

$$dX_2/dt = (Q(1 + R_1 + R_2)/V_2) (X_1^1 - X_2) + r_{X_2} \dots \quad (17)$$

Table 3 Wastewater characteristics used in the simulations (Vanhooren and Nguyen, 1996)

Variable	Value
S_H^a	30
S_{Si}^a	70
X_H^a	52
X_{Si}^a	200
X_{BHi}^a	28
X_{BAi}^a	0.25
X_{Pi}^a	5.0
S_{Oi}^b	0.25
S_{NOi}^c	0.25
S_{NHi}^c	30.0
S_{NDi}^c	7.0
X_{NDi}^c	11.0
S_{ALKi}^d	10.0

a: mg COD/L, mg of Chemical Oxygen Demand; b: mg O₂/L; c: mg N/L; d: mol/L

Table 4 Kinetic and stoichiometric parameters used in the simulation (Alex *et al.*, 2008)

Parameter	Definition	Value
μ_H	Max. specific growth rate for Heterotrophs (d ⁻¹)	4.0
μ_A	Max. specific growth rate for Autotrophs (d ⁻¹)	0.5
K_S	Half saturation constant for Heterotrophs (mg COD/L)	10
K_{OH}	Half saturation constant for O ₂ Heterotrophs (mg O ₂ /L)	0.2
K_{NO}	Half saturation constant for Heterotrophs (mg NO ₃ -N/L)	0.5
η_G	Correction for Anoxic Heterotrophic growth (-)	0.8
K_{OA}	Half saturation constant for O ₂ Autotrophs (mg O ₂ /L)	0.4
K_{NH}	Half saturation constant for Autotrophic. (mg NH ₃ -N/L)	1.0
b_H	Decay constant for Heterotrophs (d ⁻¹)	0.3
b_A	Decay constant for Autotrophs (d ⁻¹)	0.05
k_a	Ammonification rate (l.COD/mg.d)	0.05
k_h	Max. specific Hydrolysis rate (mg COD/mg COD biomass.d)	3.0
K_X	Half saturation constant for Hydrolysis (mg COD/mg COD biomass)	0.1
η_h	Correction for Anoxic Hydrolysis (-)	0.8
y_H	Heterotrophic yield coefficient (mg biomass/mg COD)	0.67
y_A	Autotrophic yield coefficient (mg biomass/mg N)	0.24
f_p	Particulate yielding biomass fraction (-)	0.08
i_{XB}	Nitrogen fraction in biomass (mg N/mg COD biomass)	0.08
i_{XP}	Nitrogen fraction in biomass products (mg N/mg COD biomass)	0.06

2. Computer simulations

The performance of the PD-AS is simulated dynamically under ideal conditions (CSTR) and real conditions (CSTR with dead volume and two CSTRs with material exchange). The characteristics of treated wastewater are given in Table 3, the kinetic and stoichiometric parameters are given in Table 4. The group of ODEs representing the behavior of all constituents in the system were solved simultaneously in order to simulate the operation of the system for 30 days. The equations were solved using fourth-order Runge-Kutta procedure in MATLAB (The MathWorks Inc., Natick, MA), with a maximum time step of 1 day. The system's performance was evaluated by calculating the following constituents in the effluent (Alex *et al.*, 2008):

- A. Total Kjeldahl Nitrogen (Rittmann and McCarty, 2001) in effluent and waste (TKN_E and TKN_W):

$$TKN_E = S_{NH}^2 + X_{ND}^{OF} + i_{XB}(X_{BA}^{OF} + X_{BH}^{OF}) + i_{XP}(X_P^{OF} + X_I^{OF}) \quad (18)$$

$$TKN_W = S_{NH}^2 + X_{ND}^{UF} + i_{XB}(X_{BA}^{UF} + X_{BH}^{UF}) + i_{XP}(X_P^{UF} + X_I^{UF}) \quad (19)$$

- B. Total Ammonia and Nitrate concentrations (S_{NH-E} and S_{NO-E}).

- C. Biochemical oxygen demanding (Rittmann and McCarty, 2001) organics in the effluent (BOD_E and BOD_W):

$$BOD_E = 0.25(S_S^2 + X_S^{OF} + (1 - f)(X_{BA}^{OF} + X_{BH}^{OF})) \quad (20)$$

$$BOD_W = 0.25(S_S^2 + X_S^{UF} + (1-f)(X_{BA}^{UF} + X_{BH}^{UF})) \quad (21)$$

D. Chemical oxygen demanding (Rittmann and McCarty, 2001) organics in effluent and waste (COD_E and COD_W):

$$COD_E = S_I^2 + S_S^2 + X_I^{OF} + X_S^{OF} + X_{BA}^{OF} + X_{BH}^{OF} + X_P^{OF} \quad (22)$$

$$COD_W = S_I^2 + S_S^2 + X_I^{UF} + X_S^{UF} + X_{BA}^{UF} + X_{BH}^{UF} + X_P^{UF} \quad (23)$$

To study the system performance under real conditions, multiple simulations were performed while varying the values of the two parameters in the real reactor models in order to reflect varying degrees of nonideal flow: For the CSTR with dead volume model, α was changed from 1 to 0.1, while β was changed from 0 to 0.9, and for the two CSTRs with exchange model α was changed from 0.9 to 0.1, while β was changed from 0.01 to 0.9. The aforementioned values for α and β were chosen to depict a moderate, intermediate, and extreme non-ideal flow scenarios.

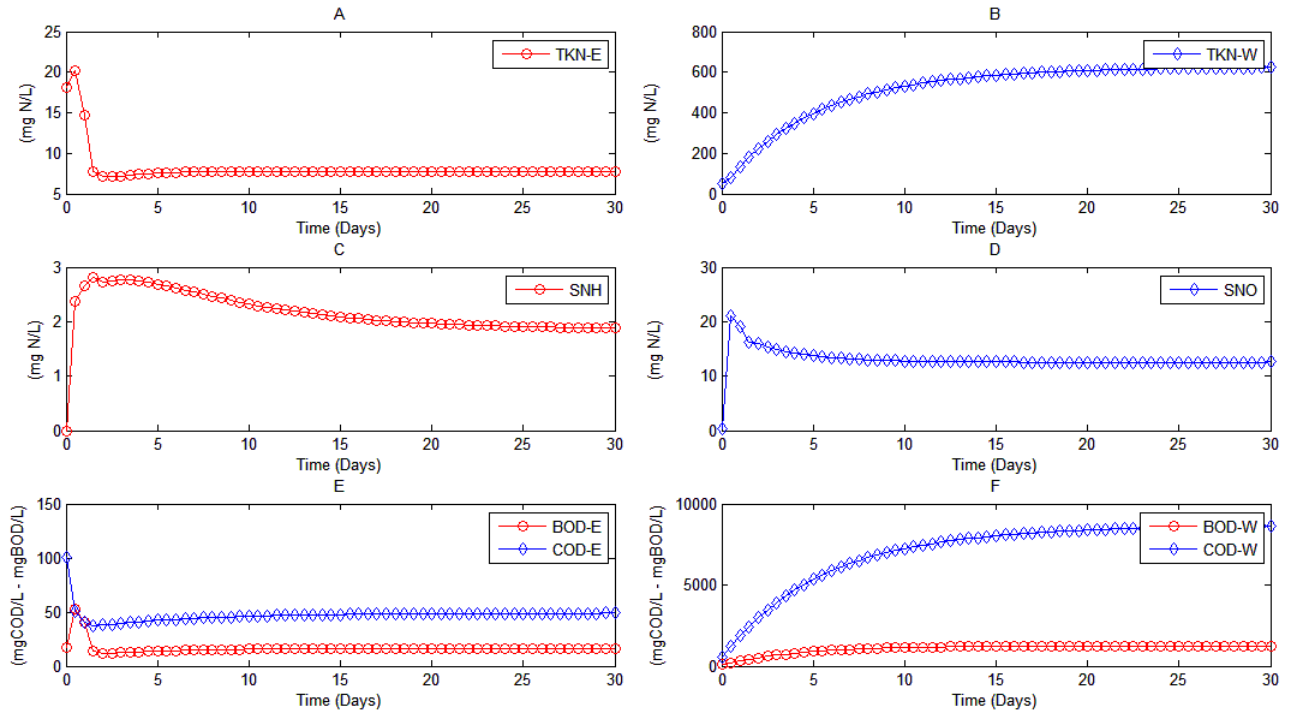


Fig. 3 PD-AS performance under ideal mixing condition; A: TKN_E , B: TKN_W , C: S_{NH-E} , D: S_{NO-E} , E: BOD_E and COD_E , and F: BOD_W and COD_W .

3 Results and Discussion

3.1 Ideal completely mixed reactors

The PD-AS system operation was simulated for 30 days. **Figure 3**, shows the system performance as a function of time. Effluent steady-state S_{NH} , S_{NO} , and TKN_E concentrations were 1.8, 12.5, and 3.9 mg N/L, respectively, while BOD_E and COD_E were 16.4 mg/L and 48.9 mg/L, respectively. The daily waste included 626 mg N/L of TKN , 1271 mg/L of BOD , and 8625 mg/L of COD . The simulation outcome was comparable to other published simulations results for similar PD-AS reactor sizes and feed wastewater composition (Alex *et al.*, 2008).

3.2 CSTR with bypass and dead volume

Figure 4 shows the effect of varying the non-ideal mixing parameters on the concentration of nitrogen compounds in the system. As can be seen, the system's effluent TKN concentration varied marginally with increasing mixing non-idealities (**Figure 4A**) (i.e. increased bypass fraction and dead volume fraction). This can be attributed to the fact that effluent TKN is mainly soluble, and removed in the aerobic reactor, where mixing performance was assumed ideal.

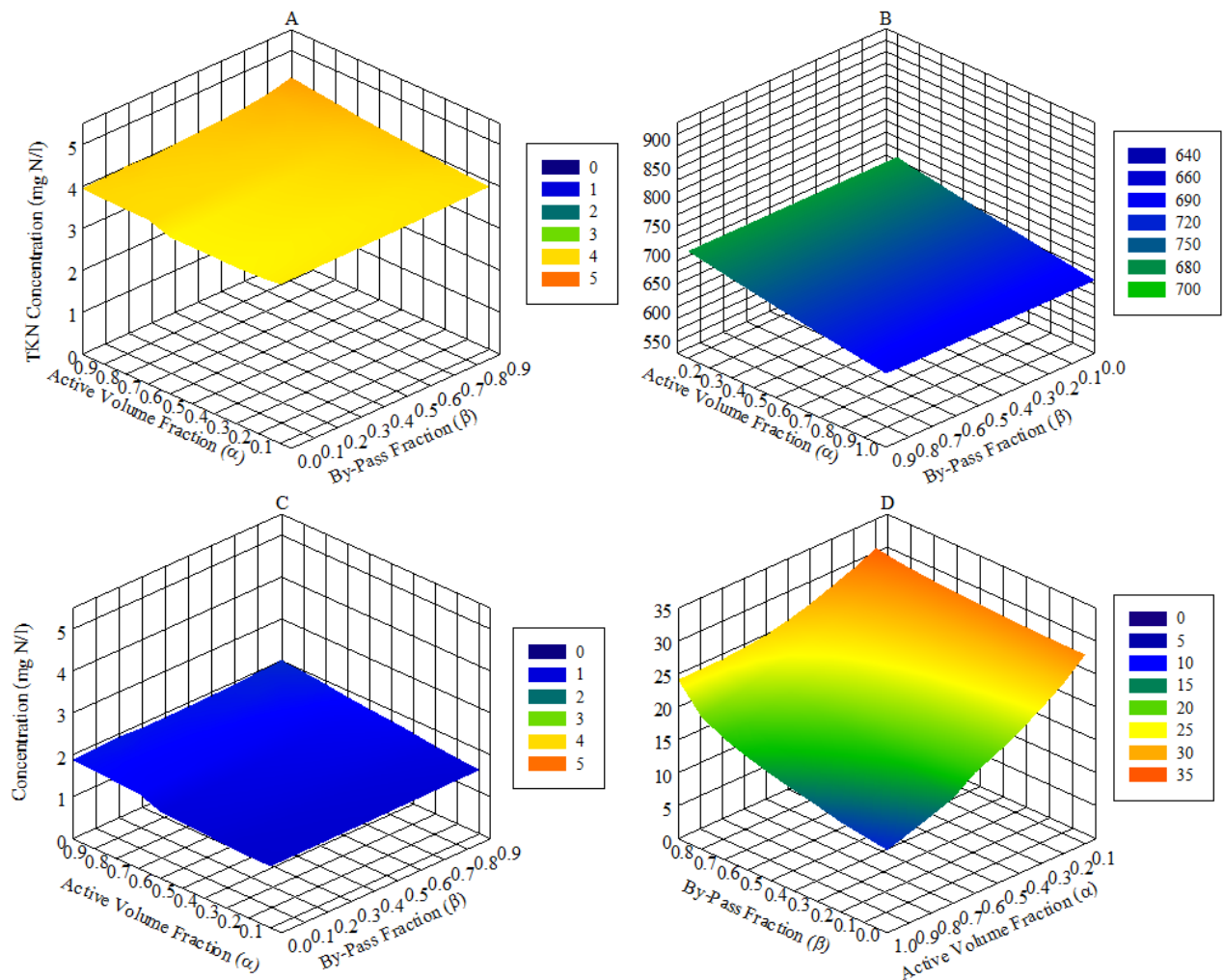


Fig. 4 Simulated PD-AS nitrogen related performance under CSTR with bypass/dead volume non-ideal mixing effects at $0.1 \leq \alpha \leq 1.0$ and $0 \leq \beta < 0.9$; A: TKN_E , B: TKN_W , C: S_{NH-E} , and D: S_{NO-E} .

The same trend was noticed for the total ammonia in the effluent, which remained relatively constant (**Figure 4C**). TKN_W increased with increasing mixing non-idealities, as can be seen in **Figure 4B**. This is attributed to the increase in the heterotrophic biomass in the system (from 2570 to 2980 mg COD/L) as a result of the increase in substrate availability in the aerobic reactor brought by the increase in bypass ratio. The TKN_W increase may affect anaerobic treatment for the wasted biomass (Chen *et al.*, 2008; Tezel *et al.*, 2014), due to the elevated levels of nitrogen. On the other hand, the effluent nitrate concentration increased drastically as the system was shifted towards non-ideal mixing conditions. As seen in Fig. 4C, S_{NO-E} exceeded 20 mg N/L at $\alpha \leq 0.4$ and $\beta \leq 0.4$. The decrease in α (increase in dead volume fraction) had a larger effect on S_{NO-E} compared to β . Similar performance short comes were observed by Manenti *et al.* (Manenti *et al.*, 2018), when the actual retention time failed in assuring an acceptable treatment level below a minimum threshold value. Collivignarelli (Collivignarelli *et al.*, 2018) reported that reducing the dead volume fraction will result in an enhancement of nitrate removal, while Kjellstr and co-researchers (Kjellstrand *et al.*, 2005) reported that the presence of a dead volume in the reactor will reduce the denitrifying capacity due to reduced active volume, and high nitrate concentration in the effluent can appear due to the short-circuiting stream (bypass). **Figure 5** shows the effect of varying the non-ideal mixing parameters on the concentration of BOD and COD in the system. As seen in **Figure 5A** and **Figure 5B**, increasing mixing non-idealities had a slight effect on BOD_E and COD_E . However, as with S_{NO-E} , decreasing α had the main effect. This can be attributed to the reduction in the anoxic reactor's active volume size, leading to a lesser conversion due to smaller real retention times (Fogler, 1999). This connects to the increase in S_{NO-E} as seen in **Figure 4D** since (as mentioned in section 1) nitrite is utilized exclusively by the heterotrophic biomass organic carbon mineralization in the anoxic reactor.

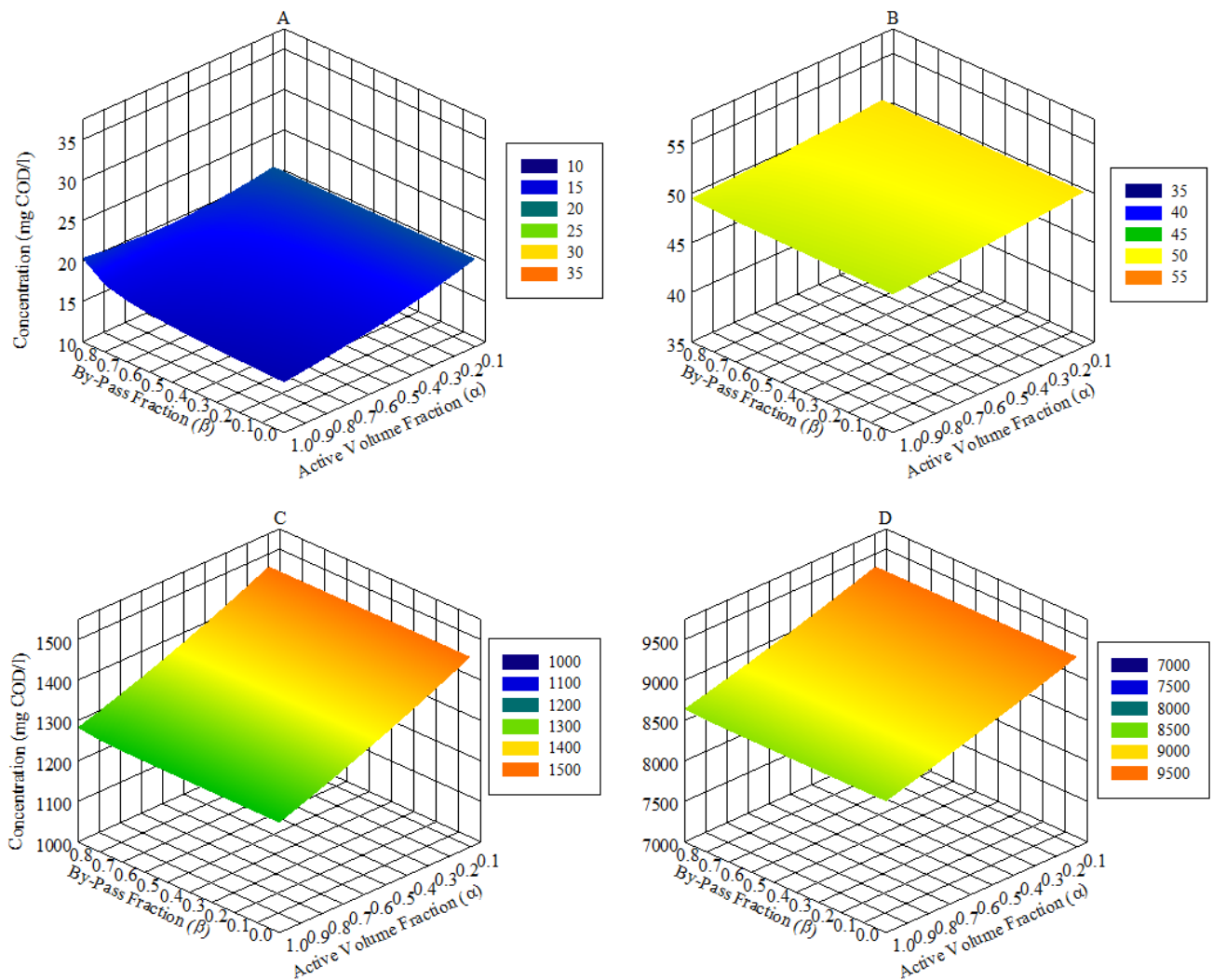


Fig. 5 Simulated PD-AS organic carbon-related performance under CSTR with bypass/dead volume non-ideal mixing effects at $0.1 \leq \alpha \leq 1.0$ and $0 \leq \beta < 0.9$; A: BOD_E , B: COD_E , C: BOD_W , and D: COD_W .

As seen in Fig. 5C and Fig. 5D, both of BOD_W and COD_W concentrations increased in the waste stream as a direct response to increased biomass in the system, which was brought by the greater than before availability of substrate in the aerobic reactor due to increased bypass fraction and decreased active volume fraction in the anoxic reactor. Collivignarelli (Collivignarelli *et al.*, 2018) reported that reducing the dead volume fraction will enhance COD and BOD. The increase in the concentrations of BOD_W and COD_W in the waste stream, coupled with the increase of TKN_W , will amplify the load on waste disposal facilities in the wastewater treatment plant. Similar to what has been observed with S_{NO-E} above, the active volume fraction (α) had a larger effect on the system's BOD and COD concentrations when compared to the bypass fraction. It must be added that, apart from nitrate concentration, the resulting changes in the PD-AS's performance were related to particulate constituents in the system. However, their concentration in the system is directly correlated with the settler's performance (i.e. SE value). The SE value was assumed constant to eliminate the effect of the settler's performance on the predicted outcome.

3.3 Two CSTRs with material exchange

As mentioned in section 2.3.2, this model describes a scenario where the mixing apparatus in the anoxic reactor are poorly positioned, resulting in rapid mixing in their vicinity, while the remaining region undergoes mixing, albeit at a lesser rate. Carried out simulations for the system's operation at the current non-ideal mixing scenario showed that, to some extent, its performance was unaffected. This was in a specific range of the mixing model α and β values: $0.4 \leq \alpha \leq 0.9$ and $0.1 \leq \beta \leq 0.9$. Table 5 shows the unaffected system's performance. **Figure 6** and **Figure 7** shows the performance of the system beyond the abovementioned range for the mixing model parameters values (i.e. second range at $0.1 \leq \alpha < 0.4$ and $0.01 \leq \beta < 0.1$). It is clear that the system's effluent TKN concentration slightly (**Figure 6A**) varied with increasing mixing non-idealities within the second range (i.e. reducing the rapid agitation zone and material exchange fractions). This took place because TKN is mainly removed in the aerobic reactor, which its mixing performance was assumed ideal. The relatively constant total ammonia in the effluent (**Figure 6C**) suggests that that ammonia removal is

unaffected.

Table 5 Effluent constituents of the PD-AS system with and without ideal mixing conditions

Effluent Constituents	Ideal mixing	CSTRs with material exchange
TKN_E	3.9 mg N/L	3.9 ± 0.09^a mg N/L
TKN_W	626.5 mg N/L	628.5 ± 4.8 mg N/L
S_{NH-E}	1.9 mg N/L	1.8 ± 0.05 mg N/L
S_{NO-E}	12.6 mg N/L	14.1 ± 1.2 mg N/L
BOD_E	16.2 mg BOD/L	16.7 ± 0.9 mg BOD/L
COD_E	48.9 mg COD/L	49.1 ± 0.2 mg COD/L
BOD_W	1271.9 mg BOD/L	1278.8 ± 15.2 mg BOD/L
COD_W	8625.6 mg COD/L	8652.3 ± 61.5 mg COD/L

a: Average \pm Standard Deviation.

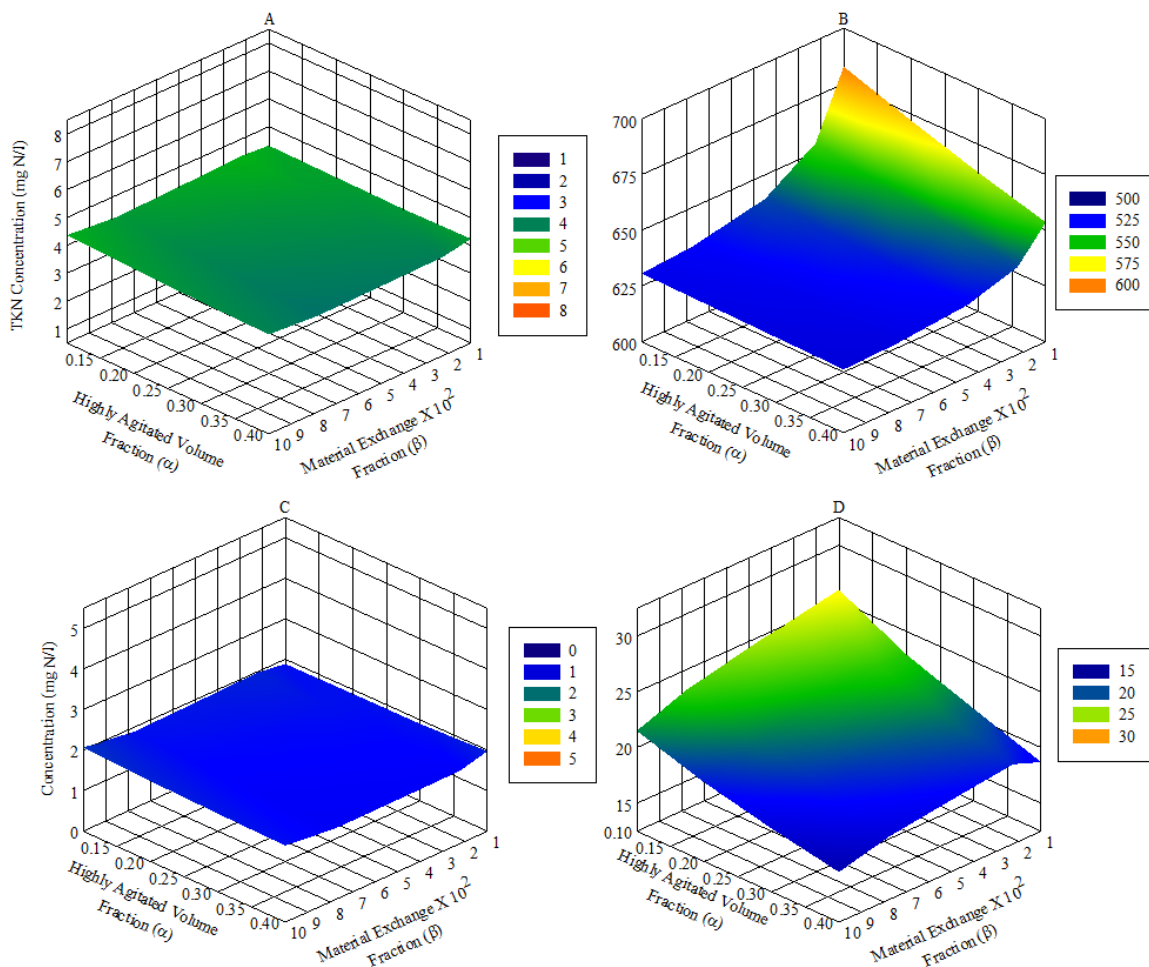


Fig. 6 Simulated PD-AS nitrogen related performance under the 2 CSTRs with material exchange non-ideal mixing effects at $0.1 \leq \alpha < 0.4$ and $0.01 \leq \beta < 0.1$; A: TKN_E , B: TKN_W , C: S_{NH-E} , and D: S_{NO-E} .

However, the TKN_W (which is mainly comprised from particulates) increased with increasing mixing non-idealities (**Figure 6B**), but only at extreme non-ideal mixing condition, when the anoxic reactor volume was mostly affected by low mixing due to very slow agitation ($\alpha < 0.3$ and $\beta < 0.01$). Operation within this range also increased the heterotrophic biomass in the system (from 2570 to 2708 ± 136 mg COD/L), due to ineffective utilization of readily biodegradable organic carbon in the anoxic reactor ($S_S + X_S$ increased in

the anoxic reactor effluent from 82.2 to 117 ± 12 mg COD/L), and were utilized by the aerobic reactor. Similar to the dead volume/bypass model, the increase TKN_W concentration and biomass concentration in the waste stream may affect anaerobic treatment processes for the wasted biomass. The effluent nitrate concentration increased drastically as the system was shifted towards extreme non-ideal mixing conditions. As seen in Fig. 6C, S_{NO-E} exceeded 20 mg N/L at $\alpha < 0.2$ and $\beta < 0.01$. This behavior mimicked the result seen in the dead volume/bypass model, however at more extreme non-ideal mixing conditions in this model. The increase is probably a result of the anoxic reactor's active volume becoming extremely low (i.e. fast residence times), not permitting any effective reactions. This can be connected to the increase of readily biodegradable organic carbon in the anoxic reactor (see before), being not utilized fully under these conditions. Results shown in Fig. 6 showed that the system's performance was more affected by the high agitation fraction (α). Fig. 7 shows the effect of varying the nonideal mixing parameters on the concentration of BOD and COD in the system.

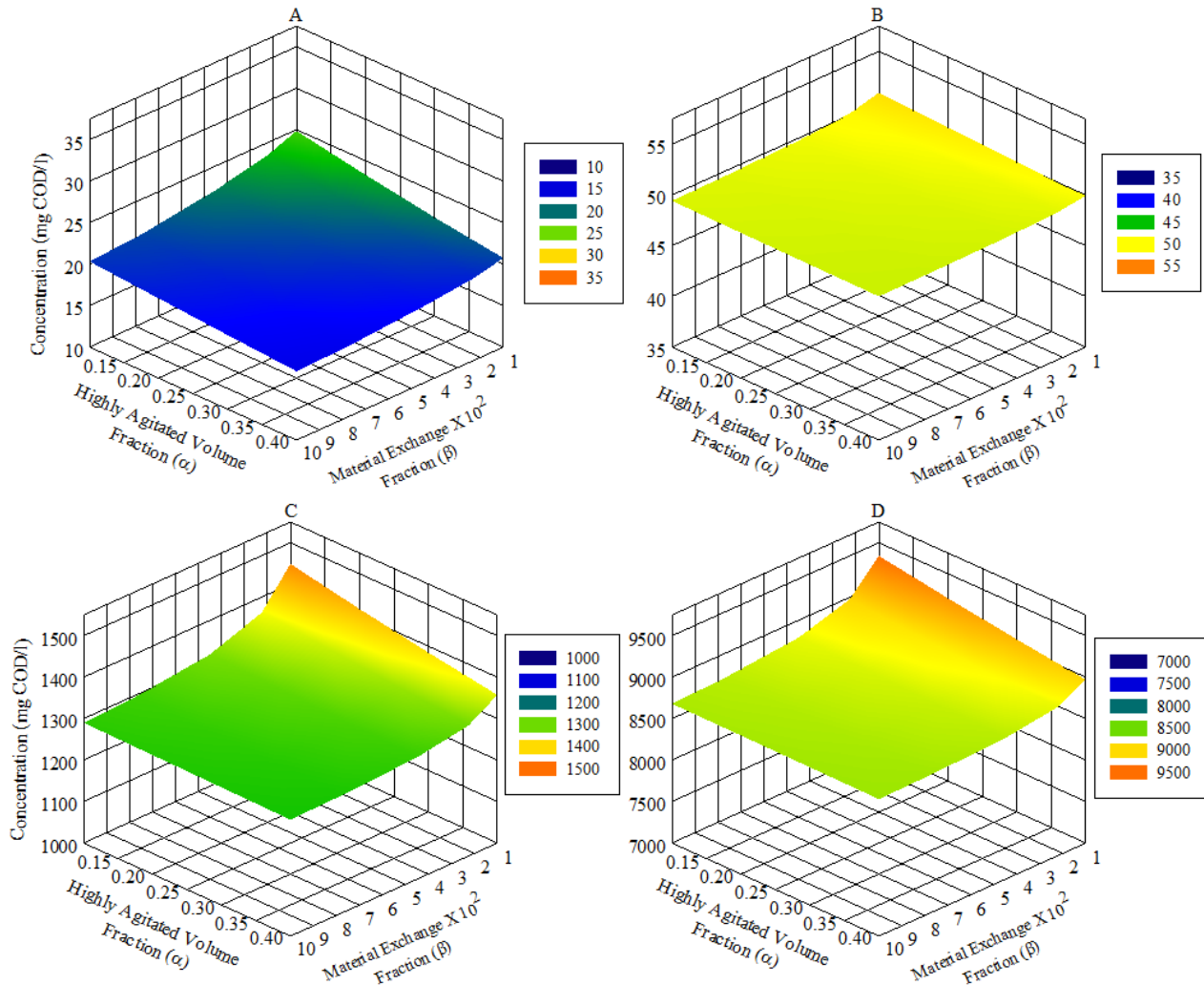


Fig. 7 Simulated PD-AS nitrogen related performance under the 2 CSTRs with material exchange non-ideal mixing effects at $0.1 \leq \alpha < 0.4$ and $0.01 \leq \beta < 0.1$; A: TKN_E , B: TKN_W , C: S_{NH-E} , and D: S_{NO-E} .

As seen in Fig. 7.A and Fig. 7.B, only extreme levels of mixing non-idealities had an effect on BOD_E and COD_E . The increase is probably related to the increased heterotrophic biomass in the system (from 2570 to 2708 ± 136 mg COD/L), due to ineffective utilization of readily biodegradable organic carbon in the anoxic reactor. As seen in Fig. 7.C and Fig. 7.D, both of BOD_W and COD_W concentrations increased in the waste stream as a direct response to increased biomass in the system, which was brought by the greater than before availability of substrate in the aerobic reactor due to reduced active anoxic reactor volume. The increase in the concentrations of BOD_W and COD_W in the waste stream will amplify the load on waste disposal facilities in the wastewater treatment plant. The aforementioned results showed that the system's performance was more affected by the high agitation fraction (α). Results shown in Figs. 6 and 7 showed that the non-ideal mixing scenario depicted by the two CSTRs with the material exchange had minor effects on the performance of the PD-AS system. Even so, these effects occurred at extreme non-ideal situations. However, this stipulation could be related to the specific operating conditions of the PD-AS under investigation. Moreover, previously published work suggests that increasing the number of CSTRs (i.e. compartments) in this model could provide a more representative depiction of the mixing non-idealities in AS systems (Liotta *et al.*, 2014).

Conclusions

The system's performance was largely affected by the presence of a dead volume/bypass scenario compared to the two mixing zones with a material exchange scenario. Under non-ideal mixing conditions, effluent concentrations of Total Kjeldahl Nitrogen, organic carbon increased marginally. On the other hand, the effluent concentration of nitrate increased significantly under the same conditions, indicating a reduction in nitrate removal efficiency. The heterotrophic biomass concentration in the system increased under non-ideal mixing conditions. This by its part resulted in an increase in the waste stream concentrations of Total Kjeldahl Nitrogen and organic carbon. This study provides an insight into the behavior of pre-denitrification activated sludge systems when affected by non-ideal mixing conditions. Additionally, it identified some performance discrepancies that could-if found in a real system-indicate the presence of a dead volume/bypass or two mixing zones mixing non-idealities in the anoxic reactor.

Nomenclature

Acronyms

AS	=Activated Sludge
PD	=Pre-Denitrification
CSTR	=Continuous stirred-tank reactor
SE	=particulates separation coefficient
COD	=Chemical Oxygen Demand
BOD	=Biochemical Oxygen Demand
TKN	=Total Kjeldahl Nitrogen
E	=Effluent
W	=Waste
UF	=Underflow
OF	=Overflow

Symbols

S	=Dissolved material concentration	[mg COD/L]
S_i	=Dissolved material concentration in the feed	[mg COD/L]
S_I	=Soluble inert organics concentration	[mg COD/L]
S_S	=Readily biodegradable (soluble) substrate concentration	[mg COD/l]
X	=particulate material concentration	[mg COD/L]
X_i	=Particulate material concentration in the feed	[mg COD/L]
X_I	=Particulate inert organics concentration	[mg COD/L]
X_S	=Slowly biodegradable (particulate) concentration	[mg COD/L]
X_{BH}	=Active heterotrophic biomass concentration	[mg COD/L]
X_{BA}	=Active autotrophic biomass concentration	[mg COD/L]
X_P	=Non-biodegradable particulates from cell decay concentration	[mg COD/L]
S_O	=Dissolved oxygen concentration	[mg O ₂ /L]
S_O^{SAT}	=Saturation dissolved oxygen concentration	[mg O ₂ /L]
S_{NO}	=Nitrate concentration	[mg N/L]
S_{NH}	=Free and ionized ammonia concentration	[mg N/L]
S_{ND}	=Soluble biodegradable organic nitrogen concentration	[mg N/L]
X_{ND}	=Particulate biodegradable organic nitrogen concentration	[mg N/L]
S_{ALK}	=Alkalinity	[mol/L]
K_L	=Oxygen transfer coefficient	[d ⁻¹]
Q	=Feed wastewater flow rate	[m ³ /d]
Q_W	=Waste flow rate	[m ³ /d]
R_I	=Nitrate recycle ratio	[-]
R_2	=Solids recycle ratio	[-]
V_I	=Anoxic reactor volume	[m ³]
V_2	=Aerobic reactor volume	[m ³]
r	=Reaction rate	[mg/L.d]
K_S	=Half saturation constant for Heterotrophs	[mg COD/L]
K_{OH}	=Half saturation constant for O ₂ Heterotrophs	[mg O ₂ /L]
K_{NO}	=Half saturation constant for Heterotrophs	[mg NO ₃ -N/L]
K_{OA}	=Half saturation constant for O ₂ Autotrophs	[mg O ₂ /L]
K_{NH}	=Half saturation constant for Autotrophic	[mg NH ₃ -N/L]
b_H	=Decay constant for Heterotrophs	[d ⁻¹]
b_A	=Decay constant for Autotrophs	[d ⁻¹]
k_a	=Ammonification rate	[L.mg COD/mg.d]
k_h	=Max. specific Hydrolysis rate	[mg COD/mg COD.d]
K_X	=Half saturation constant for Hydrolysis	[mg COD/mg COD]
y_H	=Heterotrophic yield coefficient	[mg biomass/mg COD]
y_A	=Autotrophic yield coefficient	[mg biomass/mg N]
f_p	=Particulate yielding biomass fraction	[-]
i_{XB}	=Nitrogen fraction in biomass	[mg N/mg COD biomass]
i_{XP}	=Nitrogen fraction in biomass products	[mg N/mg COD biomass]

Greek letters

α	=Non-ideal mixing parameter 1	[-]
β	=Non-ideal mixing parameter 2	[-]
μ_H	=Max. specific growth rate for Heterotrophs	[d ⁻¹]
μ_A	=Max. specific growth rate for Autotrophs	[d ⁻¹]
η_G	=Correction for Anoxic Heterotrophic growth	[-]
η_h	=Correction for Anoxic Hydrolysis	[-]

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